

AMENDMENTS TO THE CLAIMS

1. (Currently Amended) A molecular stereochemical coding ~~method for taking~~ computer program containing program instructions executable by a computer and capable of causing said computer to take a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, said ~~method~~ instructions comprising:

~~a hierarchy classifying step of~~ atoms in a hierarchy by assigning a start atom, which is to be ~~noticed~~ coded, to a zero-th ~~hierarchy serving~~ hierarchical level as the lowest hierarchy, assigning an another atom, which is ~~combined with~~ bonded to said start atom ~~on a higher hierarchy side,~~ to a first ~~hierarchy~~ hierarchical level, assigning an atom, which is ~~combined with~~ bonded to said another atom assigned to said first ~~hierarchy~~ hierarchical level, to a second ~~hierarchy~~ hierarchical level, and similarly, sequentially assigning atoms to ~~hierarchies~~ hierarchical levels until the a final hierarchy which is set so as to be specially requested is made in a form which may be accessed by a processor;

~~a molecular tree forming step of setting~~ forming a molecular tree with a predetermined precedence rule ~~for placing a plurality of atoms, which belong to the same hierarchy, in the order, and by~~ placing said atoms, which belong to the same ~~hierarchy~~ hierarchical

level, in the an order every ~~hierarchy~~ in accordance with said precedence rule, to form a molecular tree wherein every ~~said~~ start atom from a lower ~~hierarchy~~ hierarchical level to a higher ~~hierarchy~~ hierarchical level ~~so as to~~ is expressed in a bonding relationship between said plurality of atoms;

a coding ~~step of noticing~~ one of atoms, which are was assigned to the (n+3)-th ~~hierarchy~~ hierarchical level, ~~with respect to each of integers n assuming that~~ wherein n is an integer of 0 or more, in said molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th ~~hierarchy~~ hierarchical level, an atom in the (n+2)-th ~~hierarchy~~ hierarchical level and an atom in the (n+1)-th ~~hierarchy~~ hierarchical level, and a theoretical plane, which is formed by the atom in the (n+2)-th ~~hierarchy~~ hierarchical level, the atom in the (n+1)-th ~~hierarchy~~ hierarchical level and an atom in the n-th ~~hierarchy~~ hierarchical level, with respect to a group comprising four atoms which consists of said coded ~~the noticed~~ atom in the (n+3)-th ~~hierarchy~~ hierarchical level, the atom in the (n+2)-th ~~hierarchy~~ hierarchical level which is bonded to ~~combined with~~ the atom in the (n+3)-th ~~hierarchy~~ hierarchical level, the atom in the (n+1)-th ~~hierarchy~~ hierarchical level which is bonded to ~~combined with~~ the atom in the (n+2)-th ~~hierarchy~~ hierarchical level, and the atom in the n-th ~~hierarchy~~ hierarchical level which is bonded to

~~combined with~~ the atom in the (n+1)-th hierarchy hierarchical level, replacing the derived dihedral angle ~~into~~ with an angular symbol, ~~which is defined in accordance with a predetermined~~ an angle dividing rule, ~~in accordance with~~ based on the magnitude of the dihedral angle, ~~giving~~ assigning the replaced angular symbol to the ~~noticed~~ coded atom in the (n+3)-th hierarchy hierarchical level, and similarly, ~~giving~~ assigning angular symbols ~~in accordance with~~ based on the magnitudes of the dihedral angles with respect to other atoms to be ~~noticed~~ coded; and

~~setting with~~ a ~~predetermined~~ linear notation rule, ~~for~~ expressing said molecular tree by a row of characters, carrying out the linear notation of a set of ~~said plurality of~~ angular symbols in accordance with said ~~predetermined~~ linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms.

2. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, which further comprises ~~a configuration code preparing step of~~ instructions for preparing a configuration code indicative of a configuration of the molecule for every ~~said~~ start atom, and

~~wherein said configuration code preparing step causes coding~~
~~an atom, which is to be noticed in the n-th hierarchy, to be~~
~~positioned at hierarchical level by assigning said atom as a~~
~~reference position in said angle dividing rule, integrally rotates~~
~~rotating~~ all of ~~said the~~ atoms belonging to the (n+3)-th ~~hierarchy~~
hierarchical level around a bonding axis, which connects the atom
in the (n+1)-th ~~hierarchy~~ hierarchical level to the atom in the
(n+2)-th ~~hierarchy~~ hierarchical level, so that an atom, which has a
~~predetermined~~ precedence in accordance with said precedence rule
among said atoms belonging to the (n+3)-th ~~hierarchy~~ hierarchical
level, is positioned at a ~~predetermined~~ an angular position with
respect to said reference position, ~~gives~~ giving an angular symbol
according to said angle dividing rule to each of said atoms
belonging to the (n+3)-th ~~hierarchy~~ hierarchical level, in
accordance with an angular position after rotation with respect to
said reference position, ~~earries~~ carrying out the linear notation
of a set of said plurality of angular symbols in accordance with
said ~~predetermined~~ linear notation rule so as to correspond to said
molecular tree, and prepares a configuration code for every ~~said~~
start atom.

3. (Currently Amended) ~~A molecular stereochemical coding~~
~~method~~ The computer program as set forth in claim 1 or 2, which

further comprises a ~~planar structure code preparing step of~~
instructions for preparing a planar structure code indicative of a
planar structure of the molecule for every ~~said~~ start atom, and

wherein ~~said planar structure code preparing step expresses~~
said molecular tree is expressed by a set of planar structure
symbols which planar-structurally express a bonding relationship
between said plurality of atoms, ~~carries~~ carrying out the linear
notation of said set of planar structure symbols in accordance with
said ~~predetermined~~ linear notation rule so as to correspond to said
molecular tree, ~~prepares~~ preparing a planar structure code
indicative of the planar structure of the molecule with respect to
said start atom, and similarly, ~~prepares~~ preparing planar structure
codes with respect to other start atoms.

4. (Currently Amended) ~~A molecular stereochemical coding~~
~~method~~ The computer program as set forth in claim 3, wherein said
conformation codes, said configuration codes and said planar
structure codes are expressed in parallel with respect to said
start atoms.

5. (Currently Amended) ~~A molecular stereochemical coding~~
~~method~~ The computer program as set forth in claim 2, wherein when
it is impossible to rotate said atoms belonging to the (n+3)-th
~~hierarchy~~ hierarchical level around the bonding axis connecting the

atom belonging to the (n+1)-th ~~hierarchy~~ hierarchical level to the atom belonging to the (n+2)-th ~~hierarchy~~ hierarchical level, said angular symbols given at said coding step are adopted as they are, and the linear notation of a set of said plurality of angular symbols is carried out in accordance with said ~~predetermined~~ linear notation rule so as to correspond to said molecular tree, to prepare said configuration codes for every ~~said~~ start atom.

6. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 3, wherein said planar structural codes are CANOST linear notations.

7. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, wherein said precedence rule is a CANOST code precedence rule.

8. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, wherein said ~~predetermined~~ linear notation rule is a CANOST code linear notation rule.

9. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, wherein ~~at~~ during the formation of said molecular tree ~~forming step~~, a group of atoms having a low degree of ~~not ice~~ coding in the identification

of stereochemistry are replaced with ~~predetermined~~ symbols to be masked.

10. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, wherein said ~~predetermined~~ angle dividing rule divides an angle of 360 degrees into a ~~predetermined~~ number of clock-dial-like angular ranges, and the divided angular ranges are reflected in the level of abundance to be unequally divided.

11. (Currently Amended) ~~A molecular stereochemical coding method~~ The computer program as set forth in claim 1, wherein ~~at~~ during the preparation of said conformation codes ~~preparing step~~, said conformation codes are prepared with respect to at least two of said start atoms, the ~~hierarchy~~ hierarchical level numbers of which are spaced from each other by three ~~hierarchy~~ hierarchical levels or more.

12. (Currently Amended) A computer readable recording media, in which a program for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule has been recorded, said program comprising:

~~a hierarchy classifying step of~~ classifying atoms in a hierarchy by assigning a start atom, which is to be ~~noticed~~ coded,

to a zero-th ~~hierarchy~~ hierarchical level, assigning an another atom, which is ~~combined with~~ bonded to said start atom ~~on a higher hierarchy side,~~ to a first ~~hierarchy~~ hierarchical level, assigning an atom, which is ~~combined with~~ bonded to said another atom assigned to said first ~~hierarchy~~ hierarchical level, to a second ~~hierarchy~~ hierarchical level, and similarly, sequentially assigning atoms to ~~hierarchies~~ hierarchical levels until ~~the~~ a final hierarchy ~~which is set so as to be specially requested~~ is made in a form which may be accessed;

~~a molecular tree forming step of setting~~ forming a molecular tree with a predetermined precedence rule ~~for placing a plurality of atoms, which belong to the same hierarchy, in the order, and by~~ placing said atoms, which belong to the same ~~hierarchy~~ hierarchical level, in the an order ~~every hierarchy~~ in accordance with said precedence rule, to form a molecular tree wherein every said start atom from a lower ~~hierarchy~~ hierarchical level to a higher ~~hierarchy~~ hierarchical level ~~so as to~~ is expressed in a bonding relationship between said plurality of atoms;

a coding ~~step of noticing~~ one of atoms, which are was assigned to the (n+3)-th ~~hierarchy~~ hierarchical level, ~~with respect to each of integers n assuming that~~ wherein n is an integer of 0 or more, in said molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th

~~hierarchy~~ hierarchical level, an atom in the (n+2)-th ~~hierarchy~~ hierarchical level and an atom in the (n+1)-th ~~hierarchy~~ hierarchical level, and a theoretical plane, which is formed by the atom in the (n+2)-th ~~hierarchy~~ hierarchical level, the atom in the (n+1)-th ~~hierarchy~~ hierarchical level and an atom in the n-th ~~hierarchy~~ hierarchical level, with respect to a group comprising four atoms which consists of said coded ~~the noticed~~ atom in the (n+3)-th ~~hierarchy~~ hierarchical level, the atom in the (n+2)-th ~~hierarchy~~ hierarchical level which is bonded to ~~combined with~~ the atom in the (n+3)-th ~~hierarchy~~ hierarchical level, the atom in the (n+1)-th ~~hierarchy~~ hierarchical level which is bonded to ~~combined with~~ the atom in the (n+2)-th ~~hierarchy~~ hierarchical level, and the atom in the n-th ~~hierarchy~~ hierarchical level which is bonded to ~~combined with~~ the atom in the (n+1)-th ~~hierarchy~~ hierarchical level, replacing the derived dihedral angle ~~into~~ with an angular symbol, ~~which is defined~~ in accordance with a ~~predetermined~~ an angle dividing rule, ~~in accordance with~~ based on the magnitude of the dihedral angle, ~~giving~~ assigning the ~~replaced~~ angular symbol to the ~~noticed~~ coded atom in the (n+3)-th ~~hierarchy~~ hierarchical level, and similarly, ~~giving~~ assigning angular symbols ~~in accordance with~~ based on the magnitudes of the dihedral angles with respect to other atoms to be ~~noticed~~ coded; and

~~setting~~ with a ~~predetermined~~ linear notation rule, ~~for~~ expressing said molecular tree by a row of characters, carrying out ~~the~~ linear notation of a set of ~~said plurality of~~ angular symbols in accordance with said ~~predetermined~~ linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms.

13. (New) A computer readable medium containing instructions, executed by a processor, for performing a method for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, said method comprising:

classifying atoms in a hierarchy by assigning a start atom, which is to be coded, to a zero-th hierarchical level, assigning another atom, which is bonded to said start atom to a first hierarchical level, assigning an atom, which is bonded to said another atom assigned to said first hierarchical level, to a second hierarchical level, and similarly, sequentially assigning atoms to hierarchical levels until a final hierarchy is made in a form which may be accessed;

forming a molecular tree with a precedence rule by placing said atoms, which belong to the same hierarchical level, in an

order in accordance with said precedence rule to form a molecular tree wherein every start atom from a lower hierarchical level to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms;

coding one atom, which was assigned to the $(n+3)$ -th hierarchical level, wherein n is an integer of 0 or more, in said molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the $(n+3)$ -th hierarchical level, an atom in the $(n+2)$ -th hierarchical level and an atom in the $(n+1)$ -th hierarchical level, and a theoretical plane, which is formed by the atom in the $(n+2)$ -th hierarchical level, the atom in the $(n+1)$ -th hierarchical level and an atom in the n -th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the $(n+3)$ -th hierarchical level, the atom in the $(n+2)$ -th hierarchical level which is bonded to the atom in the $(n+3)$ -th hierarchical level, the atom in the $(n+1)$ -th hierarchical level which is bonded to the atom in the $(n+2)$ -th hierarchical level, and the atom in the n -th hierarchical level which is bonded to the atom in the $(n+1)$ -th hierarchical level, replacing the derived dihedral angle with an angular symbol in accordance with an angle dividing rule based on the magnitude of the dihedral angle, assigning the angular symbol to the coded atom in the $(n+3)$ -th hierarchical level, and similarly, assigning

angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; and

with a linear notation rule, expressing said molecular tree by a row of characters, carrying out linear notation of a set of angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms,

wherein the codes of the molecule are recorded in a computer readable recording medium to give the stereochemistry about each of a plurality of atoms constituting the molecule.

14. (New) The computer program as set forth in claim 1, further comprising calculating NMR shifts based upon said conformation codes.

15. (New) The computer program as set forth in claim 14, wherein the NMR shifts are printed on computer readable recording media.

16. (New) The computer program as set forth in claim 2, further comprising printing the conformation code and configuration code of the molecule on computer readable recording media.

17. (New) The computer readable recording media according to claim 12, wherein the computer readable recording media contains said program which is a set of instructions, executed by a processor, for performing said program for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, and

wherein the codes of the molecule are recorded in a computer readable recording medium to give the stereochemistry about each of a plurality of atoms constituting the molecule.